O_2
Gas phase Energy: -150.3166227 hartrees
Solvation Energy: 0.00000031291 hartrees
Zero Point Energy: 2.374 kcal/mol
Free Energy: -12.537 kcal/mol

	angstroms		
atom	x	y	z
O1	0.0000000000	0.0000000000	-0.0570704056
O2	0.0000000000	0.0000000000	1.1570704056

HOAc
Gas phase Energy: -248.28710977095 hartrees
Solvation Energy: -0.00416394432 hartrees
Zero Point Energy: 55.807 kcal/mol
Free Energy: -16.784 kcal/mol

	angstroms		
atom	x	y	z
O1	-1.9242327516	-0.2037125857	-0.0059903323
C2	-2.4789843812	1.0352746496	0.0002616290
O3	-1.8114638113	2.0450217046	0.0071373623
C4	-3.9851556595	0.9647599284	-0.0012609790
H5	-4.3335448793	0.4224117372	0.8828620818
H6	-4.3326577106	0.4125618917	-0.8794681116
H7	-4.3971755009	1.9731175821	-0.0063777995
H8	-0.9622994749	-0.0638393625	-0.0033214622

Pyridine
Gas phase Energy: -229.08745121225 hartrees
Solvation Energy: -0.00678691404 hartrees
Zero Point Energy: 38.903 kcal/mol
Free Energy: -17.003 kcal/mol

	angstroms		
atom	x	y	z
H1	-2.0604512337	-0.0000042197	0.8201907716
N2	0.0000246171	0.0000011229	0.7063155684
C3	1.1422189400	-0.0000000950	1.4048792637
C4	1.1983761625	-0.0000005443	2.7995907817
C5	-0.0000570897	-0.0000000308	3.5119582658
C6	-1.1984794598	0.0000002963	2.7996709138
C7	-1.1420705593	-0.0000003234	1.4050498252
H8	2.0606183809	0.0000004752	0.8197539303
H9	2.1570177646	-0.0000033567	3.3093019062
H10	-0.0001334952	-0.0000006072	4.5982452634
H11	-2.1572504988	0.0000008619	3.3091957661

OOH

Gas phase Energy: -150.90085005895 hartrees
Solvation Energy: -0.00535019357 hartrees
Zero Point Energy: 8.864 kcal/mol
Free Energy: -13.923 kcal/mol

angstroms

atom	x	y	z
H1	0.0903646611	0.0000000000	0.0494563780
O2	-0.0850528388	0.0000000000	1.0129913814
O3	1.1185895282	0.0000000000	1.5838924172

1
Gas phase Energy: -852.45725421632 hartrees
Solvation Energy: -0.01409351433 hartrees
Zero Point Energy: 151.565 kcal/mol
Free Energy: -30.858 kcal/mol

angstroms

atom	x	y	z
Pd1	0.0582756583	-0.0307461819	-0.0058944792
N2	0.0828492742	-0.0790560730	2.0726829105
C3	1.1874088436	0.1624280841	2.8070962222
C4	1.1776371181	0.1229729134	4.1968245794
C5	-0.0112486613	-0.1836398597	4.8570265365
C6	-1.1514253697	-0.4342011477	4.0966349898
C7	-1.0701881997	-0.3704891685	2.7091248126
H8	2.0865930854	0.3885602657	2.2496787140
H9	2.0919676465	0.3281822942	4.7433239465
H10	-0.0475132945	-0.2247908671	5.9414949962
H11	-2.1010015680	-0.6734233890	4.5636340634
H12	-1.9241948307	-0.5275759239	2.0585594590
N13	0.0770990222	-0.0782976522	-2.0844338034
C14	1.1695881524	0.2038217323	-2.8220965803
C15	1.1537151022	0.1759177199	-4.2121195096
C16	-0.0284379640	-0.1623263827	-4.8689664677
C17	-1.1561388530	-0.4551382380	-4.1050610320
C18	-1.0695037403	-0.4003071466	-2.7175404241
H19	2.0642086698	0.4534626254	-2.2672830514
H20	2.0580481900	0.4150052184	-4.7614769388
H21	-0.0692982949	-0.1949494382	-5.9535553157
H22	-2.1002729810	-0.7198015648	-4.5693589018
H23	-1.9156564035	-0.5869471688	-2.0648445454
H24	1.5918669237	-0.2409106890	-0.0085491281
O25	-2.1139081786	0.1115490400	-0.0032968649
C26	-2.5447201906	1.3443065741	-0.0366489874
O27	-1.8313445537	2.3486039592	-0.0687002929
C28	-4.0711996185	1.4696289169	-0.0327426802
H29	-4.4857361134	1.0121033894	0.8721870860

H30	-4.4988944161	0.9303178944	-0.8847770658
H31	-4.3661745140	2.5192905311	-0.0781217886

2
Gas phase Energy: -852.44531922894 hartrees
Solvation Energy: -0.01145314714 hartrees
Zero Point Energy: 150.661 kcal/mol
Free Energy: -30.085 kcal/mol

	angstroms		
atom	x	y	z
Pd1	0.0116197849	-0.0332358963	0.0040790460
N2	0.0076624127	-0.0234887881	2.0610107448
C3	1.0835001436	-0.0498399649	2.8701848804
C4	0.9507700746	-0.0568437418	4.2532190760
C5	-0.3180382077	-0.0329680795	4.8207208650
C6	-1.4259714754	-0.0077374886	3.9786819202
C7	-1.2249131523	-0.0053825341	2.6074140257
H8	2.0616346842	-0.0771078517	2.4031352646
H9	1.8431457623	-0.0830526842	4.8644633514
H10	-0.4435810753	-0.0366188751	5.8967886364
H11	-2.4353797648	0.0077558548	4.3699857649
N12	4.3283222201	-0.5365769318	1.9282282826
C13	5.4758016930	-0.4922058174	2.6232452608
C14	6.6993278344	-0.9369046493	2.1228306848
C15	6.7349233984	-1.4565231040	0.8268973235
C16	5.5484918868	-1.5075053048	0.0906987066
C17	4.3765702837	-1.0377702499	0.6830645397
H18	5.4156098764	-0.0799719042	3.6298748635
H19	7.5970998144	-0.8752114066	2.7353317144
H20	7.6683118452	-1.8129963921	0.4006263303
H21	5.5246399431	-1.9009274501	-0.9223944306
H22	3.4310755729	-1.0516952554	0.1442988860
H23	-2.0504738030	0.0048968338	1.9064349840
H24	1.5115865486	0.2046014875	0.0151485367
O25	-0.3771866365	-0.0990750426	-2.0415359311
C26	-1.6409699195	-0.2717290280	-1.8776493902
O27	-2.1346466806	-0.3327851366	-0.7149789804
C28	-2.5107985131	-0.3875176860	-3.1047245761
H29	-2.1091610984	-1.1529072220	-3.7735605619
H30	-2.4997904036	0.5619727128	-3.6493691892
H31	-3.5342055105	-0.6354712066	-2.8218758565

3
Gas phase Energy: -604.15114283016 hartrees
Solvation Energy: -0.01060631443 hartrees
Zero Point Energy: 94.365 kcal/mol

Free Energy: -25.517 kcal/mol

angstroms

atom	x	y	z
Pd1	-0.1919953210	-0.0073217819	-0.1121302188
N2	0.1464916868	-0.0852264542	1.9191200903
C3	1.2500624055	0.5767385653	2.3281869320
C4	1.6334897493	0.6214026994	3.6635554324
C5	0.8545328524	-0.0388904296	4.6132001704
C6	-0.2843013098	-0.7213492633	4.1884096540
C7	-0.6080292329	-0.7236651770	2.8356783830
H8	1.8178679982	1.0718185770	1.5463018687
H9	2.5281877260	1.1663754079	3.9443891740
H10	1.1297726380	-0.0217250513	5.6633695749
H11	-0.9211321704	-1.2494090099	4.8899071101
H12	-1.4812025429	-1.2385623194	2.4566490166
H13	-1.4508326589	-0.8455197171	0.0706094000
O14	-0.1848831921	0.2970880937	-2.1761614603
C15	0.8944456824	0.9938714565	-2.1464589567
O16	1.4857044517	1.2113276479	-1.0481614959
C17	1.4212984295	1.5719400442	-3.4371788492
H18	1.0958727195	0.9728567745	-4.2893467221
H19	1.0295042300	2.5879750460	-3.5589742920
H20	2.5110895981	1.6320539496	-3.4009620716

4

Gas phase Energy: -852.44940475446 hartrees

Solvation Energy: -0.01754871427 hartrees

Zero Point Energy: 151.022 kcal/mol

Free Energy: -31.825 kcal/mol

angstroms

atom	x	y	z
Pd1	-0.1771011400	-0.1283817634	-0.2199344260
N2	0.1260482622	0.1802316964	2.0278760756
C3	1.2616390432	0.6102422000	2.6010156596
C4	1.3881030989	0.8081612805	3.9732493559
C5	0.2882520304	0.5465541227	4.7897404926
C6	-0.8927809480	0.1016018553	4.1988736887
C7	-0.9352835312	-0.0662564442	2.8161896499
H8	2.0932139883	0.8034199236	1.9302485814
H9	2.3271512487	1.1623007831	4.3862157974
H10	0.3507474446	0.6904413622	5.8644380428
H11	-1.7750810851	-0.1105094171	4.7939943420
H12	-1.8295438737	-0.3867284151	2.2899869948
N13	1.8659272078	-0.1617682706	-0.6714124132
C14	2.6385163867	-1.2281794941	-0.3856725377
C15	4.0011043554	-1.2575614343	-0.6652319592

C16	4.5916417267	-0.1452541040	-1.2634875396
C17	3.7917344079	0.9563578586	-1.5641595991
C18	2.4351309367	0.9102612043	-1.2586748824
H19	2.1342351299	-2.0682406623	0.0775739875
H20	4.5803295039	-2.1404943352	-0.4166620696
H21	5.6525203744	-0.1384940403	-1.4939467113
H22	4.2040731869	1.8431183673	-2.0331021453
H23	1.7691848537	1.7357600612	-1.4821507296
H24	-0.4535587938	-0.3531980089	-1.7067965899
O25	-2.1934644006	-0.1677475140	0.1108536930
C26	-2.8121713321	0.9571426293	-0.1568409892
O27	-2.2862657338	1.9945509061	-0.5507178141
C28	-4.3209154087	0.8701295318	0.0790277591
H29	-4.5317952858	0.5391707250	1.1012476499
H30	-4.7609857767	0.1293954204	-0.5962488683
H31	-4.7818357203	1.8435823330	-0.0951009368

5

Gas phase Energy: -604.10953961625 hartrees
Solvation Energy: -0.01578663187 hartrees
Zero Point Energy: 93.683 kcal/mol
Free Energy: -26.67 kcal/mol

angstroms

atom	x	y	z
Pd1	0.0032322610	0.0371592178	-0.1151058541
N2	-0.0361471501	0.0191726263	2.1402764185
C3	1.1292681494	-0.2397125857	2.7606565132
C4	1.2415277274	-0.2859757114	4.1479998996
C5	0.1080857714	-0.0547006567	4.9254862972
C6	-1.1008199135	0.2154768032	4.2847082090
C7	-1.1266184718	0.2412972401	2.8935262691
H8	1.9734808099	-0.4158164059	2.1007467001
H9	2.2025327169	-0.5020516250	4.6030148753
H10	0.1640380857	-0.0855013287	6.0096967214
H11	-2.0100533322	0.4010684663	4.8465345817
H12	-2.0506820035	0.4442056512	2.3582746900
H13	0.0869040244	0.0491410344	-1.6311024822
O14	1.9422895210	-0.6175150828	-0.1839514069
C15	2.0344075280	-1.8752191404	-0.5595377628
O16	1.1023699069	-2.6077051274	-0.8614735881
C17	3.4845700757	-2.3637902796	-0.5601806938
H18	4.1077917590	-1.7052360400	-1.1708247748
H19	3.8872556738	-2.3438272331	0.4576915038
H20	3.5233529529	-3.3828348144	-0.9459902876

6_{trip}

Gas phase Energy: -1002.77629877311 hartrees
Solvation Energy: -0.01207698217 hartrees
Zero Point Energy: 154.111 kcal/mol
Free Energy: -34.9 kcal/mol

angstroms

atom	x	y	z
Pd1	0.0941410236	-0.3954956699	0.0837737694
N2	0.0574958393	-0.4215979603	2.1597622681
C3	1.1669415127	-0.2925237506	2.9134257687
C4	1.1220383940	-0.2705006677	4.3029912910
C5	-0.1107234114	-0.3952896153	4.9416710060
C6	-1.2566111431	-0.5295230051	4.1603055367
C7	-1.1374217646	-0.5335861363	2.7741028612
H8	2.0995749636	-0.2011803489	2.3719132868
H9	2.0428325732	-0.1574183773	4.8654611234
H10	-0.1759554167	-0.3842400054	6.0256940281
H11	-2.2390463710	-0.6232237569	4.6105038627
H12	-1.9916730256	-0.5941073175	2.1083943276
N13	0.1617599213	-0.4064753086	-1.9929839217
C14	1.3110853750	-0.3165220534	-2.6908044419
C15	1.3359116058	-0.2875853085	-4.0805968572
C16	0.1325633579	-0.3627565804	-4.7800501467
C17	-1.0547333447	-0.4573536873	-4.0568021094
C18	-1.0046903839	-0.4719652951	-2.6663649780
H19	2.2184589934	-0.2628304000	-2.1037549550
H20	2.2870701275	-0.2075794634	-4.5961837088
H21	0.1213530501	-0.3446168302	-5.8659019565
H22	-2.0164877851	-0.5124714497	-4.5555744461
H23	-1.8920966069	-0.5062794338	-2.0431867143
H24	1.5425900857	-0.9425424910	0.1183114193
O25	-1.9928740136	0.2095694972	0.0359082607
C26	-2.1448334630	1.5057064127	0.0604589882
O27	-1.2297689220	2.3308911730	0.1050648309
C28	-3.6062621411	1.9616595140	0.0263108073
H29	-4.1590115478	1.5264476053	0.8656326216
H30	-4.0901638808	1.6071149098	-0.8902552886
H31	-3.6661371100	3.0502511704	0.0722110728
O32	2.4033881560	2.2534361015	0.5266532244
O33	2.4135937596	2.3142462880	-0.6844877963

7_{trip}
Gas phase Energy: -1002.78875115491 hartrees
Solvation Energy: -0.01060218034 hartrees
Zero Point Energy: 155.468 kcal/mol
Free Energy: -34.519 kcal/mol

angstroms

atom	x	y	z
Pd1	0.2164678888	-0.2241260221	-0.0110655843
N2	0.2421039242	-0.3862062351	2.1313163428
C3	1.3828493239	-0.2958738946	2.8394695885
C4	1.4142257968	-0.4388639089	4.2231405266
C5	0.2197596862	-0.6793958718	4.9010994156
C6	-0.9639509955	-0.7595859697	4.1687190122
C7	-0.9139381452	-0.6056404937	2.7862038916
H8	2.2804754066	-0.0870112648	2.2673642275
H9	2.3581843651	-0.3568511375	4.7516551559
H10	0.2111810759	-0.7945993574	5.9807906810
H11	-1.9176994844	-0.9339495735	4.6557222238
H12	-1.8014802682	-0.6310366254	2.1623918608
N13	0.2283793577	-0.3840886719	-2.1537964760
C14	1.3659279039	-0.3917458485	-2.8728700335
C15	1.3762615155	-0.5741324536	-4.2524425746
C16	0.1625232709	-0.7511849245	-4.9156550664
C17	-1.0171908950	-0.7301499397	-4.1730394075
C18	-0.9455017480	-0.5422530693	-2.7956817257
H19	2.2828693700	-0.2396031048	-2.3133515338
H20	2.3191378945	-0.5740137881	-4.7892777203
H21	0.1368815515	-0.8970746919	-5.9914007139
H22	-1.9846723712	-0.8550538537	-4.6481007929
H23	-1.8266962895	-0.4954867816	-2.1638353521
H24	0.3122792961	2.4428550118	0.1907303519
O25	-2.0412614293	0.4050976091	-0.0055475279
C26	-2.1104334420	1.6740451401	0.0208813521
O27	-1.1447221406	2.4869272566	0.0664117120
C28	-3.5149155148	2.2749125609	-0.0232206080
H29	-4.1480439975	1.8010423751	0.7325294654
H30	-3.9681523699	2.0663981313	-0.9983596387
H31	-3.4841487026	3.3536718054	0.1354519144
O32	1.3422455478	2.6413127981	0.3155884364
O33	1.9960769558	1.4969844691	0.1646038504

8_{trip}

Gas phase Energy: -1002.78038818254 hartrees
Solvation Energy: -0.01620457338 hartrees
Zero Point Energy: 156.039 kcal/mol
Free Energy: -34.939 kcal/mol

angstroms

atom	x	y	z
Pd1	0.0573756633	0.0051446933	-0.0914316841
N2	0.0378519620	-0.1170671900	2.2174928985
C3	0.9461976231	0.5360837274	2.9625149103
C4	0.8252525745	0.6615281458	4.3449495465

C5	-0.2743048533	0.0857947226	4.9793182686
C6	-1.2163416377	-0.5920048473	4.2064413833
C7	-1.0273403461	-0.6663717207	2.8283101597
H8	1.7902626764	0.9486566865	2.4184520257
H9	1.5804488739	1.2035558096	4.9048807215
H10	-0.3970674936	0.1668514612	6.0554705217
H11	-2.0896174406	-1.0528775065	4.6567097372
H12	-1.7485251359	-1.1454232358	2.1744758375
N13	-0.0749702708	-0.0626782502	-2.3673679634
C14	0.9980590341	0.2480731557	-3.1129296755
C15	0.9427594716	0.2932238568	-4.5041498629
C16	-0.2641288740	0.0044976498	-5.1393796395
C17	-1.3744080135	-0.3214014949	-4.3611468073
C18	-1.2397030951	-0.3430063754	-2.9752873857
H19	1.9071067690	0.4531526929	-2.5551186093
H20	1.8312133334	0.5521754114	-5.0707622158
H21	-0.3390401782	0.0334596066	-6.2225543452
H22	-2.3324397563	-0.5544661103	-4.8140413770
H23	-2.0670915970	-0.5815995787	-2.3139368461
H24	2.8892372271	-0.7722324226	1.1559617158
O25	-2.3656743826	-0.2720607430	0.0292115661
C26	-2.4370018992	0.9904572620	0.1011835699
O27	-1.3963721333	1.7223812497	0.0642354259
C28	-3.7915354596	1.6631044077	0.2330748061
H29	-4.3149894706	1.2629939801	1.1068586502
H30	-4.4020490199	1.4296507755	-0.6450769616
H31	-3.6858777142	2.7448292717	0.3277976821
O32	3.0042271398	0.0671649948	0.6813191609
O33	2.0918203680	-0.0931963379	-0.4135769768

8_{sing}

Gas phase Energy: -1002.82389311988 hartrees
Solvent Energy: -0.01535894583 hartrees
Zero Point Energy: 157.54 kcal/mol
Free Energy: -32.382 kcal/mol

angstroms

atom	x	y	z
Pd1	-0.0062478829	0.0019389108	-0.0308872041
N2	0.0327335794	0.0658384653	2.0585503817
C3	1.1682538662	0.4138953220	2.6920620258
C4	1.2408496091	0.4714292222	4.0799929306
C5	0.1121144430	0.1525659002	4.8322942069
C6	-1.0581949674	-0.2116025595	4.1674609364
C7	-1.0629742288	-0.2406360098	2.7770371986
H8	2.0101073339	0.6253353553	2.0425467183
H9	2.1730493476	0.7600680346	4.5534411747

H10	0.1435105578	0.1867937453	5.9172557683
H11	-1.9603948239	-0.4697267889	4.7116452901
H12	-1.9407415016	-0.4979290045	2.1952699695
N13	0.0283039867	-0.0369507916	-2.1274034868
C14	1.1571693277	0.2852002125	-2.7863624631
C15	1.2046317343	0.3407439128	-4.1755790439
C16	0.0535108301	0.0469554400	-4.9046091319
C17	-1.1093516086	-0.2937008723	-4.2152127243
C18	-1.0869801955	-0.3218858971	-2.8247665878
H19	2.0188488331	0.4765730278	-2.1545220850
H20	2.1324079195	0.6116135042	-4.6685588808
H21	0.0622249193	0.0830670379	-5.9898785037
H22	-2.0281001999	-0.5318071015	-4.7404662203
H23	-1.9584853986	-0.5605137763	-2.2262452757
H24	2.4199298822	-1.8628359026	-0.4059394345
O25	-2.0853986498	0.0000741196	-0.0149797013
C26	-2.6267565542	1.1953865118	-0.1024801311
O27	-2.0073560981	2.2476198914	-0.2283278385
C28	-4.1530703695	1.1684384087	-0.0356545994
H29	-4.4821882440	0.7409958665	0.9172472448
H30	-4.5583263921	0.5309113150	-0.8281682033
H31	-4.5479707390	2.1801342707	-0.1384099028
O32	2.4180957406	-1.3572453129	0.4224856025
O33	1.9918372285	-0.0487549989	-0.0404363852

9_{trip}

Gas phase Energy: -1002.76714755705 hartrees
Solvation Energy: -0.0155590261 hartrees
Zero Point Energy: 153.652 kcal/mol
Free Energy: -33.651 kcal/mol

angstroms

atom	x	y	z
Pd1	0.0424921123	-0.3772598226	-0.2224067597
N2	0.0033514315	0.1944086164	2.0126565530
C3	1.0708730439	0.1749010100	2.8247501483
C4	1.0264587551	0.6106756894	4.1467742989
C5	-0.1828484050	1.0884005873	4.6529293364
C6	-1.2957816050	1.1046276152	3.8154842914
C7	-1.1634001659	0.6514216141	2.5029465180
H8	1.9948478204	-0.1992420141	2.3920284948
H9	1.9216662419	0.5790795251	4.7595513358
H10	-0.2529769042	1.4414336415	5.6782911980
H11	-2.2567712820	1.4684285529	4.1641400097
H12	-1.9856615774	0.6471097141	1.7936376100
N13	2.0575633080	-0.9709009153	-0.2913571653
C14	2.3902062072	-2.2765319239	-0.3117229194

C15	3.7038472835	-2.7111063297	-0.4515598185
C16	4.7183444838	-1.7649940701	-0.5828591172
C17	4.3760382044	-0.4143483882	-0.5628238490
C18	3.0398922753	-0.0572939656	-0.4167449027
H19	1.5682091739	-2.9756020460	-0.2194647908
H20	3.9171641934	-3.7741976387	-0.4626487580
H21	5.7518960835	-2.0745276953	-0.7004937537
H22	5.1269483096	0.3605460762	-0.6629191733
H23	2.7315928750	0.9810852702	-0.3899374175
H24	-0.0215492027	-0.7041818521	-1.7078628579
O25	-1.9289481644	0.1265296065	-0.2821678128
C26	-2.3773327248	0.8789801373	-1.2596644936
O27	-1.7284773570	1.3279509239	-2.1941585985
C28	-3.8692798323	1.1841132918	-1.1085322841
H29	-4.0531570401	1.7033706397	-0.1616839814
H30	-4.4486654881	0.2546076156	-1.0837947055
H31	-4.2053748190	1.8037469696	-1.9389803574
O32	0.8535835803	2.7359798214	-0.0720442108
O33	0.4651618043	3.2960071588	0.9359172218

10_{trip}

Gas phase Energy: -1002.79347448407 hartrees
Solvation Energy: -0.01184553991 hartrees
Zero Point Energy: 155.305 kcal/mol
Free Energy: -34.731 kcal/mol

angstroms

atom	x	y	z
Pd1	-0.1078360206	0.4011088314	-0.1144678423
N2	0.2644941114	0.2971532325	2.1029511120
C3	1.4156416436	0.7445612101	2.6376599730
C4	1.6406907436	0.7951382396	4.0096569665
C5	0.6295425321	0.3627128896	4.8681925334
C6	-0.5644249982	-0.0962053344	4.3171207645
C7	-0.7167492726	-0.1128349474	2.9307512603
H8	2.1734148382	1.0716343204	1.9322412760
H9	2.5860734644	1.1684604514	4.3902317192
H10	0.7704652879	0.3883659215	5.9448787834
H11	-1.3808827054	-0.4365464471	4.9452622841
H12	-1.6407483380	-0.4336831646	2.4500834072
N13	1.9928358701	-0.1385401386	-0.7239216270
C14	2.7058165135	-1.0778625307	-0.0771578186
C15	3.9583152579	-1.5037286894	-0.5106339935
C16	4.4986807228	-0.9345831708	-1.6631006760
C17	3.7607319456	0.0353062248	-2.3398502022
C18	2.5135696750	0.4028043027	-1.8407860857
H19	2.2461133086	-1.4924818954	0.8143191676

H20	4.4916499233	-2.2669946284	0.0462102066
H21	5.4736172635	-1.2436614332	-2.0278895117
H22	4.1374340151	0.5027385960	-3.2436680730
H23	1.8933602908	1.1357828470	-2.3457168025
H24	-2.1871045885	1.2268315648	-1.4869701150
O25	-2.3289824824	0.8432874768	-0.1898478203
C26	-3.3341278361	0.1140564385	0.2386478700
O27	-3.2905365994	-0.6127926862	1.2271976268
C28	-4.6109454518	0.2539134648	-0.5849869621
H29	-4.4145346114	0.0031116577	-1.6331489038
H30	-4.9593525089	1.2918859466	-0.5589618604
H31	-5.3877949376	-0.4019494457	-0.1908072531
O32	-0.4920221685	0.9737735855	-2.2633332473
O33	-1.7287397890	1.4234236162	-2.4582472735

10_{sing}

Gas phase Energy: -1002.8134295316 hartrees
Solvation Energy: -0.01746122463 hartrees
Zero Point Energy: 157.56 kcal/mol
Free Energy: -32.841 kcal/mol

angstroms

atom	x	y	z
Pd1	-0.2050127789	0.0069727133	-0.2699840657
N2	0.0222893228	0.0384874244	1.8648559408
C3	0.2032492743	1.1995196864	2.5209003357
C4	0.2665996761	1.2573418125	3.9104988275
C5	0.1186551074	0.0827129885	4.6451996182
C6	-0.0873074000	-1.1167014041	3.9635242974
C7	-0.1286457967	-1.0958780162	2.5732479298
H8	0.2592970920	2.0869637229	1.9056662660
H9	0.4154234643	2.2142285972	4.3989835211
H10	0.1547837220	0.1011933531	5.7303073442
H11	-0.2193319437	-2.0541380455	4.4927566758
H12	-0.2932159944	-1.9995968600	1.9956797177
N13	1.8664636414	-0.2882396690	-0.6721783184
C14	2.7705702641	-0.5979826056	0.2764929110
C15	4.1187576950	-0.7788693276	-0.0090546917
C16	4.5553562356	-0.6298467428	-1.3251175290
C17	3.6199420050	-0.3073799561	-2.3050331890
C18	2.2849657642	-0.1446453381	-1.9457374838
H19	2.3908264227	-0.7019018460	1.2852925459
H20	4.8064896960	-1.0330484021	0.7902463874
H21	5.6024856100	-0.7641180242	-1.5790412362
H22	3.9089885712	-0.1816047600	-3.3430648994
H23	1.4950260223	0.0827797442	-2.6560432547
H24	-2.2015984395	0.6140680492	-2.1638386930

O25	-2.2613761837	0.2051611818	-0.1066539126
C26	-2.7134347442	1.2818097719	0.4844672032
O27	-2.0298026989	2.1593646812	1.0121799417
C28	-4.2369432179	1.3884687614	0.4421225289
H29	-4.7032874603	0.4225777725	0.6527819551
H30	-4.5511021707	1.6918851554	-0.5630387498
H31	-4.5775168252	2.1401351212	1.1559262082
O32	-0.4951324905	-0.1386029215	-2.2134259926
O33	-1.3957211051	0.8921975719	-2.6380973974

11

Gas phase Energy: -852.45122266961 hartrees

Solvation Energy: -0.00857011757 hartrees

Zero Point Energy: 152.229 kcal/mol

Free Energy: -33.264 kcal/mol

angstroms

atom	x	y	z
Pd1	0.2426047727	-0.1487181892	0.0349602014
N2	0.1883666936	-0.0860244726	2.1097165609
C3	1.3318895788	-0.0522185394	2.8321007226
C4	1.3348697284	-0.0541322209	4.2247865910
C5	0.1246095888	-0.0904656640	4.9139561921
C6	-1.0560696059	-0.1259006697	4.1729326785
C7	-0.9819172935	-0.1222801657	2.7843551680
H8	2.2645096360	-0.0383109762	2.2763426042
H9	2.2840513412	-0.0295631206	4.7502550097
H10	0.1003239332	-0.0929728227	5.9998522121
H11	-2.0273118701	-0.1574491048	4.6560731131
H12	-1.8766203911	-0.1515912548	2.1744187735
N13	4.3091714322	-0.7042984243	1.3153049038
C14	3.9002374505	-1.1413311276	0.1149565186
C15	4.7103240905	-1.8830741522	-0.7468129042
C16	6.0098206093	-2.1871928320	-0.3449262003
C17	6.4466445916	-1.7367616663	0.9008100436
C18	5.5602657951	-1.0026377515	1.6887914936
H19	2.8753639445	-0.8876323729	-0.1628113670
H20	4.3238328809	-2.2119573601	-1.7065029824
H21	6.6694814823	-2.7637693114	-0.9877565358
H22	7.4498963651	-1.9486055777	1.2580318959
H23	5.8695524564	-0.6368119231	2.6668477378
H24	-1.4206208281	0.8101719420	-1.0188961957
O25	0.2572504042	-0.1967541873	-2.1138554562
C26	-0.7023275603	0.3459724064	-2.6693976369
O27	-1.6768830211	0.9289710046	-1.9888716363
C28	-0.8611218472	0.3989901440	-4.1618137686
H29	-0.0179835284	-0.0965655444	-4.6417545004

H30	-1.7968604448	-0.0889387106	-4.4511001191
H31	-0.9207901943	1.4409123986	-4.4903100720

12
Gas phase Energy: -604.15755681106 hartrees
Solvation Energy: -0.00710734654 hartrees
Zero Point Energy: 96.052 kcal/mol
Free Energy: -24.844 kcal/mol

angstroms

atom	x	y	z
Pd1	-0.1027244512	-0.1527602439	0.0083283954
N2	-0.0127540962	0.0144178657	2.0695781020
C3	1.1598516542	0.2618885999	2.6948027286
C4	1.2803683406	0.3171653126	4.0798162039
C5	0.1496829354	0.1124682221	4.8694271697
C6	-1.0636056347	-0.1431749939	4.2320865391
C7	-1.1035671121	-0.1839101961	2.8421774028
H8	2.0145610536	0.4179441308	2.0476378776
H9	2.2495667910	0.5194977090	4.5237958729
H10	0.2121325505	0.1513528299	5.9528498574
H11	-1.9747295576	-0.3102045191	4.7973896649
H12	-2.0267829021	-0.3794782110	2.3103523404
H13	-1.3458751543	1.3459140401	-1.0239311944
O14	-0.2334901057	-0.2645941932	-2.1285211925
C15	-0.9412922153	0.5867337794	-2.6737548483
O16	-1.5839493214	1.5205767564	-1.9884898813
C17	-1.1418844771	0.6510172997	-4.1604597570
H18	-0.5980565144	-0.1607854013	-4.6419941026
H19	-2.2083400698	0.5803371053	-4.3937418314
H20	-0.7878612341	1.6149046671	-4.5383828925

13_{trip}
Gas phase Energy: -1002.78669305705 hartrees
Solvation Energy: -0.00991629604 hartrees
Zero Point Energy: 155.868 kcal/mol
Free Energy: -35.258 kcal/mol

angstroms

atom	x	y	z
Pd1	-0.0744046483	-0.0231816255	0.2860488673
N2	-0.0853955604	-0.0791830820	2.4086086415
C3	1.0482926852	-0.0541682867	3.1401263733
C4	1.0306449752	-0.0772417855	4.5315086819
C5	-0.1944526550	-0.1272963734	5.1944325339
C6	-1.3630759435	-0.1515694996	4.4356696434
C7	-1.2722064632	-0.1256571439	3.0465749671
H8	1.9872724632	-0.0181280195	2.5935068771

H9	1.9689092873	-0.0543303101	5.0761756074
H10	-0.2367922051	-0.1465522074	6.2795696193
H11	-2.3408422638	-0.1891366885	4.9042782094
H12	-2.1551285277	-0.1347363995	2.4083035902
N13	3.8063052049	-0.2393787238	1.1043603399
C14	3.1875948873	-0.0144514976	-0.0645999805
C15	3.4316794124	-0.7501048066	-1.2245991954
C16	4.3846528572	-1.7653629059	-1.1748420107
C17	5.0470673809	-2.0037012747	0.0302665177
C18	4.7174829288	-1.2213362941	1.1364607924
H19	2.4603730057	0.7969391324	-0.0774255078
H20	2.8667646593	-0.5322993934	-2.1242377649
H21	4.6053692588	-2.3621545800	-2.0546025449
H22	5.7972947976	-2.7836599762	0.1178976442
H23	5.2055853978	-1.3928416706	2.0947825316
H24	-2.1695945164	0.0120594482	-1.7362416113
O25	0.2259051149	0.0883283367	-1.9153752857
C26	-0.5890281358	0.1148422846	-2.8474802702
O27	-1.8920848570	0.0708422166	-2.7128648121
C28	-0.1369823594	0.1955428773	-4.2851063749
H29	0.9464533646	0.3175448883	-4.3376113735
H30	-0.4332601723	-0.7210892834	-4.8105804423
H31	-0.6383732759	1.0322111671	-4.7821959058
O32	-2.2298981247	-0.0601824829	-0.1859114728
O33	-3.2497306456	-0.0924625789	0.6133688606

13_{sing}

Gas phase Energy: -1002.783702196 hartrees
Solvation Energy: -0.0107501007 hartrees
Zero Point Energy: 155.335 kcal/mol
Free Energy: -35.175 kcal/mol

angstroms

atom	x	y	z
Pd1	0.0713841201	0.0400952853	0.2473102806
N2	-0.0157885728	-0.0072922164	2.3721117006
C3	1.0734601747	0.1402053116	3.1544190174
C4	0.9939801940	0.1048110489	4.5433781490
C5	-0.2472836259	-0.0902485986	5.1477744915
C6	-1.3692762317	-0.2397078526	4.3357321651
C7	-1.2198073271	-0.1920818937	2.9522596701
H8	2.0233535068	0.2808497243	2.6451327228
H9	1.8965656735	0.2281694724	5.1326579112
H10	-0.3374551206	-0.1239875459	6.2297916936
H11	-2.3571971979	-0.3916063298	4.7580125127
H12	-2.0661258093	-0.2902483329	2.2714935996
N13	3.7270371727	-0.0702818570	1.0990699069

C14	3.1845770703	0.1820032596	-0.1025205234
C15	3.2541868569	-0.6999045651	-1.1837919674
C16	3.9279917241	-1.9076302293	-1.0111865226
C17	4.5014087719	-2.1818849365	0.2301509144
C18	4.3689701455	-1.2367715501	1.2482221974
H19	2.6842924536	1.1438447476	-0.2134237836
H20	2.7645527361	-0.4428502914	-2.1157760237
H21	4.0001367333	-2.6231297602	-1.8255292114
H22	5.0340373418	-3.1101516271	0.4126056583
H23	4.7958021628	-1.4261868979	2.2317027734
H24	-1.9375191023	-0.5543022675	-1.5103262931
O25	0.2824179287	0.3053879521	-1.9106440355
C26	-0.6039678468	0.1412440746	-2.7767491392
O27	-1.7911218633	-0.3220709707	-2.5493963293
C28	-0.3305198938	0.4890575366	-4.2202656824
H29	0.6813464371	0.8756035365	-4.3388916131
H30	-0.4700108019	-0.3998603057	-4.8427705698
H31	-1.0569716904	1.2352788406	-4.5557186956
O32	-1.9393718704	-0.8215204864	-0.1411413670
O33	-2.9865671563	-0.2768567722	0.4595961914

14_{trip}

Gas phase Energy: -1002.79924908858 hartrees
Solvation Energy: -0.0115444066 hartrees
Zero Point Energy: 154.858 kcal/mol
Free Energy: -35.089 kcal/mol

angstroms

atom	x	y	z
Pd1	-0.1030835414	0.2670848367	-0.1559508477
N2	0.1308060444	-0.0354777281	2.1013200121
C3	1.1527477918	0.5247622114	2.7715519172
C4	1.2519240307	0.5023301911	4.1605823582
C5	0.2488733011	-0.1325596362	4.8920342487
C6	-0.8146501963	-0.7129571258	4.2025628162
C7	-0.8395338667	-0.6390972999	2.8110623387
H8	1.9107451895	1.0079816955	2.1620895150
H9	2.0961164785	0.9762204487	4.6510955755
H10	0.2934335622	-0.1695680007	5.9768489720
H11	-1.6205802553	-1.2131834190	4.7297920308
H12	-1.6628510044	-1.0376498218	2.2297611300
N13	2.0739560507	-0.2364771235	-0.6645705316
C14	2.8031916460	-1.0766475943	0.0892111160
C15	4.0823900903	-1.4956917455	-0.2657572625
C16	4.6328717741	-1.0269931249	-1.4583042997
C17	3.8770410594	-0.1624411558	-2.2477428001
C18	2.6036858985	0.2074863602	-1.8186718807

H19	2.3340233384	-1.4209650835	1.0057893091
H20	4.6275453596	-2.1767731100	0.3799030490
H21	5.6281555704	-1.3336097930	-1.7668805817
H22	4.2595409204	0.2225662033	-3.1874458961
H23	1.9615439597	0.8551799907	-2.4075915608
H24	-2.4025594411	1.3215615166	-1.8657776783
O25	-2.3592951952	0.2116375944	0.3708673548
C26	-3.3616360459	0.6788230061	-0.2008894599
O27	-3.3677114329	1.2747324907	-1.3487156404
C28	-4.7285758191	0.5691240457	0.4430676620
H29	-4.6483687700	0.1548095293	1.4472787791
H30	-5.3671495197	-0.0737272528	-0.1686904538
H31	-5.2007771202	1.5538828084	0.4782611235
O32	-0.2325406994	0.9322870400	-2.2047197051
O33	-1.3319291255	1.4596667286	-2.7076053294

15_{sing}

Gas phase Energy: -1002.77874005245 hartrees
Solvation Energy: -0.01859141272 hartrees
Zero Point Energy: 157.365 kcal/mol
Free Energy: -32.351 kcal/mol

angstroms

atom	x	y	z
Pd1	-0.1991037908	-0.0732222550	-0.2548395002
N2	0.0809713830	0.0812468612	1.8368855527
C3	0.2712493226	1.2924161324	2.3913707639
C4	0.3935030648	1.4560207426	3.7683852728
C5	0.2940681479	0.3396713120	4.5966813505
C6	0.0743437996	-0.9104863935	4.0185321724
C7	-0.0261508074	-0.9969764449	2.6338945798
H8	0.2915094368	2.1313021928	1.7088435473
H9	0.5499684138	2.4490081396	4.1755325558
H10	0.3776777297	0.4419755057	5.6746559363
H11	-0.0228131726	-1.8061934304	4.6227885848
H12	-0.2057531378	-1.9438968995	2.1346929747
N13	1.8739017611	-0.3648338167	-0.6344932480
C14	2.7003041052	-1.0342641850	0.1908926069
C15	4.0396584726	-1.2423965083	-0.1129695513
C16	4.5413632424	-0.7371267043	-1.3138771514
C17	3.6805332692	-0.0464209815	-2.1620746239
C18	2.3453937231	0.1261190236	-1.7975736883
H19	2.2684581973	-1.4050316217	1.1137008407
H20	4.6700048730	-1.7907832372	0.5790040431
H21	5.5841318549	-0.8844652495	-1.5803748383
H22	4.0262738139	0.3593320551	-3.1070742998
H23	1.5898887051	0.6357568709	-2.4261880148

H24	-1.5729047812	0.0413913645	-2.1610726300
O25	-2.2518522857	0.0692962384	-0.1921681603
C26	-2.7741557592	1.1347932457	0.3734002572
O27	-2.1478984136	2.0136256612	0.9599927543
C28	-4.2918180700	1.1937778124	0.2291238825
H29	-4.7449658354	0.2539677182	0.5582690426
H30	-4.5562231776	1.3307219179	-0.8244964395
H31	-4.6875604021	2.0266061277	0.8119295920
O32	-0.6155120449	-0.1325708458	-2.2614159812
O33	-0.1234993712	1.0646757341	-2.8982634686

16
Gas phase Energy: -1081.57066763246 hartrees
Solvation Energy: -0.01297038338 hartrees
Zero Point Energy: 190.928 kcal/mol
Free Energy: -36.204 kcal/mol

angstroms

atom	x	y	z
Pd1	0.1416125261	0.1113661741	-0.0378454773
N2	0.2143673719	0.0725423789	2.0469663121
C3	1.3921927816	0.3096878542	2.6658887500
C4	1.5701346235	0.1529879350	4.0359079148
C5	0.4900146690	-0.2637835900	4.8136787506
C6	-0.7291001587	-0.5006637767	4.1823872340
C7	-0.8326970971	-0.3218614088	2.8046825736
H8	2.2053633743	0.6319735445	2.0260447904
H9	2.5405304843	0.3564013926	4.4771943806
H10	0.5970824687	-0.3968166316	5.8861868188
H11	-1.6018662093	-0.8207263313	4.7422061105
H12	-1.7691934331	-0.4762700192	2.2790534154
N13	0.2339785687	0.0605781636	-2.1254272927
C14	1.2890185570	-0.5602959203	-2.6997223278
C15	1.4634355986	-0.6399991448	-4.0768628776
C16	0.5132582304	-0.0565529393	-4.9143116607
C17	-0.5784437891	0.5829688711	-4.3305790213
C18	-0.6842663321	0.6199358707	-2.9427923199
H19	2.0053055420	-1.0013314878	-2.0165565896
H20	2.3319724854	-1.1526061046	-4.4775543063
H21	0.6214787115	-0.1007275599	-5.9938386219
H22	-1.3472182952	1.0518334815	-4.9362331226
H23	-1.5226454549	1.1023918895	-2.4544894192
H24	-1.8122932404	0.9809661053	-0.0925960488
O25	-3.5908004498	-0.0469854331	1.1082300766
C26	-3.7117436126	0.8148246436	0.2570961470
O27	-2.6881963790	1.4007221293	-0.3774091430

C28	-5.0439370841	1.3584855542	-0.2121029187
H29	-5.0713437683	2.4446422305	-0.0835618361
H30	-5.8506392916	0.8933654685	0.3539538024
H31	-5.1732986033	1.1538395196	-1.2795250694

17_{trip}
Gas phase Energy: -1002.79713051253 hartrees
Solvation Energy: -0.01032907923 hartrees
Zero Point Energy: 155.96 kcal/mol
Free Energy: -36.264 kcal/mol

angstroms

atom	x	y	z
Pd1	0.2415777292	-0.1562867693	0.0265324088
N2	0.1122977985	-0.2819596248	2.1305808584
C3	1.1977974873	-0.0986511304	2.9080988975
C4	1.1667321936	-0.3061553022	4.2850269475
C5	-0.0226557337	-0.7178911187	4.8832203955
C6	-1.1475951460	-0.8993666920	4.0789201782
C7	-1.0434832508	-0.6702998501	2.7105506477
H8	2.0987599172	0.2235588135	2.3908829116
H9	2.0668780253	-0.1450937445	4.8692803437
H10	-0.0738452300	-0.8911395471	5.9543973317
H11	-2.0973294662	-1.2145471828	4.4983785056
H12	-1.8923693015	-0.7894193419	2.0449170172
N13	0.1041472944	-0.2393584714	-2.0929762685
C14	1.1727746603	-0.0010794892	-2.8781289135
C15	1.1361657556	-0.1731106547	-4.2588866694
C16	-0.0456120157	-0.6086225318	-4.8563582927
C17	-1.1544804882	-0.8488423991	-4.0461384087
C18	-1.0431610489	-0.6502703511	-2.6733693169
H19	2.0684555145	0.3347389656	-2.3666245533
H20	2.0244182571	0.0326404327	-4.8471155270
H21	-0.1024082172	-0.7550283656	-5.9310611363
H22	-2.0979403922	-1.1840149411	-4.4642260319
H23	-1.8839362512	-0.8059279135	-2.0044042129
H24	-1.4214448849	1.2969989260	-0.0432371909
O25	-3.3835891253	0.0574754048	0.1004897570
C26	-3.3224841287	1.2666902703	-0.0564467531
O27	-2.1747097366	1.9509374948	-0.1271676058
C28	-4.5287372200	2.1678195482	-0.1926296155
H29	-4.5324453587	2.9061166302	0.6150309132
H30	-5.4398909292	1.5713097143	-0.1562735436
H31	-4.4773094146	2.7197857582	-1.1358070954
O32	2.3778756098	0.7749389617	-0.2330134701
O33	3.2499520428	0.7218166954	0.6866806190

17_{sing}
Gas phase Energy: -1002.78948946336 hartrees
Solvation Energy: -0.01147736068 hartrees
Zero Point Energy: 156.103 kcal/mol
Free Energy: -35.106 kcal/mol

	angstroms		
atom	x	y	z
Pd1	0.2469549686	-0.1263966170	0.0111292203
N2	0.1012519131	-0.2403232685	2.1237644169
C3	1.1824105295	-0.0426417865	2.9033093389
C4	1.1397107341	-0.2290756534	4.2831744388
C5	-0.0535440036	-0.6322639309	4.8786088267
C6	-1.1728528326	-0.8302775605	4.0696818843
C7	-1.0583829565	-0.6230093274	2.6990008978
H8	2.0852191364	0.2694007955	2.3785599037
H9	2.0352022779	-0.0590320548	4.8719317666
H10	-0.1126763381	-0.7879616960	5.9520337287
H11	-2.1246407898	-1.1410912911	4.4877945229
H12	-1.9020492709	-0.7520048719	2.0281657486
N13	0.1088790786	-0.2327179972	-2.1209901214
C14	1.1811234547	0.0154704343	-2.8981789678
C15	1.1504991142	-0.1499766801	-4.2802402177
C16	-0.0263056662	-0.5888261043	-4.8842681212
C17	-1.1376112563	-0.8411516424	-4.0802848530
C18	-1.0329236230	-0.6498961697	-2.7058229981
H19	2.0695889517	0.3541996877	-2.3740059532
H20	2.0395616499	0.0634667064	-4.8645143529
H21	-0.0777615517	-0.7294598212	-5.9600693375
H22	-2.0765041895	-1.1811006468	-4.5048333021
H23	-1.8728060318	-0.8181291927	-2.0391086856
H24	-1.2463941959	1.4997527722	-0.0212281078
O25	-3.0958108242	0.0835759179	-0.0327645227
C26	-3.1378914946	1.3037531389	-0.0689376284
O27	-2.0538761622	2.0853104540	-0.0581448303
C28	-4.4153886065	2.1083576355	-0.1324625465
H29	-4.4717528880	2.7845262410	0.7258438363
H30	-5.2735093055	1.4369360497	-0.1371198277
H31	-4.4187338361	2.7285562698	-1.0339166055
O32	2.3067306186	0.7811000050	-0.2528947184
O33	3.1613031187	0.7856665737	0.7080468972

18
Gas phase Energy: -623.36200797332 hartrees
Solvation Energy: -0.00613151677 hartrees
Zero Point Energy: 113.507 kcal/mol
Free Energy: -26.068 kcal/mol

	angstroms		
atom	x	y	z
Pd1	-0.0933154196	-0.0142312892	0.0046385074
N2	0.0046920238	-0.0009085505	2.0807137777
C3	0.9345637680	0.7342337694	2.7301536326
C4	1.0523611808	0.7530310207	4.1162779776
C5	0.1777468755	-0.0162581807	4.8826525691
C6	-0.7855893164	-0.7769544366	4.2213421168
C7	-0.8395615852	-0.7426282385	2.8312911744
H8	1.5942969762	1.3178451297	2.0996608801
H9	1.8206888605	1.3639349861	4.5792307773
H10	0.2451013990	-0.0225580175	5.9664029184
H11	-1.4915500899	-1.3932616588	4.7686871137
H12	-1.5731656894	-1.3188660091	2.2805421064
N13	-0.1677409189	-0.0179134071	-2.0723275962
C14	0.5563313235	-0.8960015511	-2.8020006418
C15	0.5531803023	-0.9092459740	-4.1937863012
C16	-0.2285746098	0.0203045978	-4.8788749302
C17	-0.9795333978	0.9293196101	-4.1344159296
C18	-0.9232791838	0.8783112925	-2.7450732854
H19	1.1498424100	-1.6004827271	-2.2319648286
H20	1.1566330016	-1.6393336288	-4.7231541496
H21	-0.2521694468	0.0362550561	-5.9643290778
H22	-1.6050110897	1.6735420206	-4.6168571227
H23	-1.4912238411	1.5668273224	-2.1310443488

19_{trip}

Gas phase Energy: -773.69289547721 hartrees
Solvation Energy: -0.01117710598 hartrees
Zero Point Energy: 116.769 kcal/mol
Free Energy: -29.66 kcal/mol

	angstroms		
atom	x	y	z
Pd1	-0.1691906787	0.0552480863	0.0127678975
N2	0.0805314669	0.0137111280	2.1183443808
C3	1.3096740624	-0.1212354814	2.6599881155
C4	1.5256494889	-0.1783701542	4.0324294341
C5	0.4293246043	-0.0932432733	4.8908000991
C6	-0.8404278209	0.0471645525	4.3353538678
C7	-0.9775152655	0.0972585974	2.9496825935
H8	2.1351552440	-0.1840589768	1.9599282065
H9	2.5358556860	-0.2877333092	4.4132253636
H10	0.5641827971	-0.1352387250	5.9677442223
H11	-1.7245843765	0.1182306723	4.9604746273
H12	-1.9465520093	0.2082857516	2.4666268250
N13	-0.1029453333	0.0262123020	-2.1166166671

C14	1.0599048064	-0.2009230147	-2.7621866837
C15	1.1582533471	-0.2340382060	-4.1492453012
C16	0.0092850789	-0.0234060651	-4.9110908894
C17	-1.1939957349	0.2119268227	-4.2487470016
C18	-1.2110656144	0.2290975935	-2.8565125276
H19	1.9291236733	-0.3602511588	-2.1339714072
H20	2.1199494358	-0.4224231121	-4.6151833331
H21	0.0521899114	-0.0431236738	-5.9960894597
H22	-2.1156351493	0.3807703677	-4.7959084776
H23	-2.1234857202	0.4041871029	-2.2959996939
O24	-2.4506086028	0.4129126231	-0.1472515856
O25	-3.2296324605	0.4413214723	0.8587742865

19_{sing}

Gas phase Energy: -773.67012716849 hartrees
Solvation Energy: -0.01220306904 hartrees
Zero Point Energy: 117.203 kcal/mol
Free Energy: -27.939 kcal/mol

angstroms

atom	x	y	z
Pd1	-0.1379070011	0.1615089027	0.0569552924
N2	0.0654744068	0.0648431848	2.1743304731
C3	1.2672655097	0.0738663630	2.7842483173
C4	1.4090958971	-0.0334789252	4.1637195091
C5	0.2633569289	-0.1554185384	4.9498905644
C6	-0.9801184507	-0.1615547996	4.3209790489
C7	-1.0411536766	-0.0486231083	2.9346011853
H8	2.1327473919	0.1679654038	2.1368861666
H9	2.4001720371	-0.0236215600	4.6051824774
H10	0.3401954364	-0.2434914298	6.0297170042
H11	-1.8994019123	-0.2533208806	4.8900138438
H12	-1.9740045416	-0.0501103531	2.3778620814
N13	-0.1423908383	0.1024958835	-2.0723634378
C14	0.9579002096	-0.2534544449	-2.7658413606
C15	0.9592808966	-0.3944427805	-4.1488744097
C16	-0.2255019466	-0.1601176676	-4.8475684861
C17	-1.3619485017	0.2074618416	-4.1312053548
C18	-1.2890706643	0.3290649714	-2.7445055758
H19	1.8564748736	-0.4304286042	-2.1840458228
H20	1.8715046855	-0.6841191427	-4.6599824477
H21	-0.2591048008	-0.2643125282	-5.9283035263
H22	-2.3056609290	0.3978247883	-4.6317698136
H23	-2.1424007012	0.6152508804	-2.1231189119
O24	-2.1907534088	-0.0435707386	0.2187988100
O25	-2.8301117926	0.9677313975	-0.3125777731

20_{trip}
Gas phase Energy: -773.68335518056 hartrees
Solvation Energy: -0.00901864351 hartrees
Zero Point Energy: 116.012 kcal/mol
Free Energy: -32.14 kcal/mol

angstroms

atom	x	y	z
Pd1	-0.3270940295	0.3890464836	-0.0080889023
N2	-0.1670350065	0.0087453643	2.1155977089
C3	0.2877489854	0.9604568652	2.9564733054
C4	0.5130387478	0.7279297355	4.3101001628
C5	0.2582713292	-0.5409987451	4.8290340649
C6	-0.2144786603	-1.5294753899	3.9667738388
C7	-0.4136036675	-1.2153136774	2.6255003669
H8	0.4711600699	1.9333314583	2.5136181440
H9	0.8799645655	1.5322957361	4.9392895714
H10	0.4228000071	-0.7539585205	5.8808482583
H11	-0.4305199280	-2.5320615638	4.3211976365
H12	-0.7830051677	-1.9539560057	1.9226191554
N13	1.8812555444	-0.3162383022	-0.7217769837
C14	2.8198637675	-0.8197036251	0.0934672529
C15	4.0947381872	-1.1745199129	-0.3428586310
C16	4.4110123959	-0.9982753104	-1.6895952278
C17	3.4398222030	-0.4754482577	-2.5422651468
C18	2.1899574710	-0.1482249803	-2.0176169016
H19	2.5311328037	-0.9399850989	1.1344032132
H20	4.8179727130	-1.5783614225	0.3588818580
H21	5.3947250069	-1.2632683276	-2.0662607554
H22	3.6409714800	-0.3211486920	-3.5974322069
H23	1.4011640453	0.2620799477	-2.6420183109
O24	-2.0148991683	1.3687786701	-1.6764707417
O25	-0.8375790674	0.8961049649	-1.9386063952

20_{sing}
Gas phase Energy: -773.69055862913 hartrees
Solvation Energy: -0.01744463067 hartrees
Zero Point Energy: 117.156 kcal/mol
Free Energy: -28.734 kcal/mol

angstroms

atom	x	y	z
Pd1	-0.1483020602	0.0020933020	-0.1087285940
N2	0.0274218091	-0.0219093190	2.0517925154
C3	0.9704181699	-0.6814335475	2.7486237074
C4	0.9423772397	-0.7894053744	4.1360449199
C5	-0.1047496694	-0.1910805667	4.8356128625
C6	-1.0852021673	0.4926310392	4.1174719575

C7	-0.9859629483	0.5530321047	2.7310526871
H8	1.7614547291	-1.1375266594	2.1620642347
H9	1.7248427967	-1.3377176676	4.6502070543
H10	-0.1581894529	-0.2599955197	5.9177537442
H11	-1.9218091610	0.9701589262	4.6165314828
H12	-1.7311484693	1.0574949591	2.1252916850
N13	1.9417050596	0.0227710278	-0.6863275468
C14	2.9181697317	0.6820893934	-0.0366624931
C15	4.2151117764	0.7840945722	-0.5315735718
C16	4.5186027315	0.1797167808	-1.7508632723
C17	3.5092706372	-0.5031353215	-2.4285091393
C18	2.2373559957	-0.5573639409	-1.8671480164
H19	2.6344643074	1.1431868203	0.9038275906
H20	4.9650468110	1.3322238608	0.0291944489
H21	5.5195230776	0.2432442449	-2.1666513019
H22	3.6951057475	-0.9851289798	-3.3823513119
H23	1.4144358269	-1.0615441745	-2.3625327716
O24	-2.0871900665	0.0078857085	-0.6160365838
O25	-1.2999144075	0.0028918951	-1.7495877303

21
Gas phase Energy: -1081.57066763246 hartrees
Solvation Energy: -0.01297038338 hartrees
Zero Point Energy: 190.928 kcal/mol
Free Energy: -36.204 kcal/mol

angstroms

atom	x	y	z
Pd1	0.4251598498	-0.3766816651	0.0166558051
N2	0.3779247640	-0.4920330610	2.0838840926
C3	1.1467524862	0.2816984167	2.8742273233
C4	1.0766950327	0.2030865338	4.2623939892
C5	0.1906616680	-0.6973786006	4.8506196615
C6	-0.6115792670	-1.4854587208	4.0259919972
C7	-0.4942477433	-1.3522697329	2.6472228359
H8	1.7842347418	0.9944696756	2.3685883828
H9	1.7065385169	0.8508318933	4.8625821907
H10	0.1181664349	-0.7772510866	5.9314792650
H11	-1.3271696482	-2.1900735966	4.4369562783
H12	-1.1208532373	-1.9058190006	1.9581206267
N13	0.4942529088	-0.3038205453	-2.0603978885
C14	1.5488610564	0.1772750992	-2.7479376887
C15	1.5529154459	0.2605009976	-4.1359161581
C16	0.4329074582	-0.1721792695	-4.8436927122
C17	-0.6556469252	-0.6714437871	-4.1313276866
C18	-0.5920298581	-0.7196092424	-2.7427293737
H19	2.3952841902	0.4968966746	-2.1545811671

H20	2.4237048681	0.6598643010	-4.6445989305
H21	0.4088647470	-0.1187182346	-5.9281411229
H22	-1.5517572792	-1.0158835322	-4.6361234502
H23	-1.4161605203	-1.0691537045	-2.1308627741
H24	1.9642479788	-0.3948965689	0.0667039032
O25	-1.7511049866	-0.5229633089	0.0125730965
C26	-2.4488247800	0.5530167440	0.1115290585
O27	-2.0191643840	1.7227152756	0.0569147032
C28	-3.9524199981	0.3571826104	0.3009405888
H29	-4.4840471768	0.7956127754	-0.5503270530
H30	-4.2163518467	-0.6981708105	0.3918834764
H31	-4.2780642251	0.9002353466	1.1934401202
O32	1.1517872989	2.8840579813	1.2669572476
C33	1.0493752124	3.3336747703	0.1321833834
O34	0.0795140855	3.0344341089	-0.7231379737
C35	2.0327081544	4.3301724208	-0.4586957836
H36	2.3634977324	4.0032145494	-1.4463254704
H37	1.5386465110	5.2986739419	-0.5884988873
H38	2.8868509600	4.4482989234	0.2052413572
H39	-0.6268772922	2.4288135167	-0.3178795720

22
Gas phase Energy: -1081.56970582854 hartrees
Solvation Energy: -0.01052664112 hartrees
Zero Point Energy: 191.098 kcal/mol
Free Energy: -36.568 kcal/mol

angstroms

atom	x	y	z
Pd1	0.4933770160	-0.2246725860	0.1130195471
N2	0.2902191483	-0.2980971458	2.1932900308
C3	1.1748140938	0.1999811388	3.0837474959
C4	1.0263532754	0.0084546939	4.4564387903
C5	-0.0639178877	-0.7155836220	4.9338180784
C6	-0.9822493264	-1.2217945484	4.0135124738
C7	-0.7744149624	-0.9918593267	2.6589090436
H8	2.0088585350	0.7626727249	2.6724106275
H9	1.7651571739	0.4289659209	5.1306990504
H10	-0.1999799118	-0.8797133183	5.9989263085
H11	-1.8521298742	-1.7870598557	4.3330272950
H12	-1.4729159723	-1.3501127447	1.9097926243
N13	0.4849697292	-0.3889890217	-1.9736262482
C14	1.5177233212	-0.0517394127	-2.7741584764
C15	1.5298995150	-0.3251208151	-4.1389557686
C16	0.4356751506	-0.9696869349	-4.7116056630
C17	-0.6375444743	-1.3130186680	-3.8895673966
C18	-0.5796549350	-1.0079596601	-2.5334263048

H19	2.3439181777	0.4581430231	-2.2950064926
H20	2.3881453339	-0.0309334245	-4.7338453049
H21	0.4175991978	-1.1964495724	-5.7735278510
H22	-1.5151274742	-1.8119375241	-4.2862419929
H23	-1.3976447068	-1.2449837157	-1.8601937456
H24	2.0205003734	1.0935812827	-0.0145681372
O25	-2.9808725948	-0.7280420768	-0.0981411864
C26	-3.2004107382	0.4746666964	-0.0717535853
O27	-2.2442625133	1.4043614404	-0.0055868864
C28	-4.5813564681	1.0908039622	-0.1143933718
H29	-4.6707855903	1.7386779321	-0.9907336797
H30	-5.3349550723	0.3048925593	-0.1535717984
H31	-4.7381574940	1.7185278228	0.7669632037
O32	2.8216641538	1.7206014754	-0.4058263204
C33	3.5901414187	2.1630225285	0.5176330703
O34	3.4725998003	1.9305344082	1.7260416180
C35	4.7143913692	3.0383130819	-0.0083410730
H36	5.3089808128	3.4127751528	0.8248211604
H37	5.3493472021	2.4609476907	-0.6862854598
H38	4.3031603261	3.8757544674	-0.5797143999
H39	-1.3515482613	0.9550018622	0.0281421492

TS6-7
Gas phase Energy: -1002.75275684933 hartrees
Solvation Energy: -0.01266787376 hartrees
Zero Point Energy: 151.927 kcal/mol
Free Energy: -34.816 kcal/mol

angstroms

atom	x	y	z
Pd1	0.0858426763	-0.2097122276	0.1284226608
N2	0.0578393789	-0.2968314470	2.2183297213
C3	1.1744927306	-0.2030564129	2.9668912578
C4	1.1441162397	-0.2942567186	4.3547480934
C5	-0.0786415301	-0.4894234634	4.9935179826
C6	-1.2322528192	-0.5797958600	4.2159731025
C7	-1.1294773325	-0.4764801291	2.8324955340
H8	2.1099210616	-0.0600483585	2.4346177343
H9	2.0707025579	-0.2141146193	4.9134346232
H10	-0.1312332381	-0.5672339442	6.0755352789
H11	-2.2071270533	-0.7267257197	4.6683585544
H12	-1.9882167012	-0.5158447388	2.1702987491
N13	0.1835939281	-0.2751763867	-1.9675204352
C14	1.3218803705	-0.0916574490	-2.6644652015
C15	1.3623595992	-0.1550387511	-4.0530828741
C16	0.1856779017	-0.4196787377	-4.7511487928
C17	-0.9923867923	-0.6032889074	-4.0292708732

C18	-0.9588742559	-0.5206602388	-2.6408154088
H19	2.2169232604	0.1036906358	-2.0861894820
H20	2.3049086094	0.0002962924	-4.5672733184
H21	0.1871876927	-0.4785186141	-5.8355710537
H22	-1.9338942590	-0.8059245574	-4.5283763246
H23	-1.8441658152	-0.6245894136	-2.0223064118
H24	1.7444710405	-0.4717757250	0.1616670339
O25	-2.1252714534	0.1607434832	0.0604604872
C26	-2.2536551343	1.4543079254	0.0076023580
O27	-1.3191255320	2.2634890514	-0.0000520909
C28	-3.7029081827	1.9448155902	-0.0389650158
H29	-4.2162651739	1.6703170153	0.8890750659
H30	-4.2416506201	1.4603612706	-0.8595770045
H31	-3.7306963644	3.0285798169	-0.1628677951
O32	3.0200866292	-0.6207052200	-0.0278039974
O33	3.7033284824	-0.2878636397	0.9956177015

TS9-10
Gas phase Energy: -1002.74655591435 hartrees
Solvation Energy: -0.01494530788 hartrees
Zero Point Energy: 151.318 kcal/mol
Free Energy: -36.513 kcal/mol

angstroms

atom	x	y	z
Pd1	0.0013259567	0.0635073724	0.1870716112
N2	-0.0601432736	-0.0705529781	2.5023918170
C3	0.9712107776	-0.3935130083	3.2963960841
C4	0.8546328145	-0.4940866464	4.6800892163
C5	-0.3878298713	-0.2485927568	5.2645239772
C6	-1.4602266763	0.0906309088	4.4416583361
C7	-1.2559898833	0.1712910264	3.0656870531
H8	1.9198267397	-0.5753948179	2.7984763106
H9	1.7197544043	-0.7572141852	5.2800046175
H10	-0.5160815746	-0.3188515936	6.3407710824
H11	-2.4445832806	0.2925197353	4.8515383174
H12	-2.0452498447	0.4394929873	2.3682579336
N13	1.9214053586	-0.7307527608	-0.1661413762
C14	2.2569761961	-1.9956117979	0.1559445408
C15	3.4779019654	-2.5580665157	-0.1998664162
C16	4.3926679671	-1.7860474565	-0.9162353206
C17	4.0474336429	-0.4785265546	-1.2506091873
C18	2.8032767629	0.0112931053	-0.8652174866
H19	1.5112206629	-2.5587586283	0.7069602879
H20	3.6974867835	-3.5838678130	0.0765411203
H21	5.3523193730	-2.1985545612	-1.2130185363
H22	4.7207036482	0.1582758911	-1.8142569080

H23	2.4824946636	1.0149198809	-1.1209052427
H24	-0.1235255487	0.0577227101	-1.4449634233
O25	-1.9232582252	0.8142614067	0.2157988384
C26	-1.9440196607	2.0156541523	-0.3015032483
O27	-0.9444914461	2.6260803498	-0.6869635288
C28	-3.3391423224	2.6156049725	-0.4273062177
H29	-3.9120638924	2.4718182448	0.4930889266
H30	-3.8798520100	2.1036444953	-1.2308789833
H31	-3.2698361028	3.6779026274	-0.6663931963
O32	-0.1957827041	-0.0392026893	-2.7762057596
O33	0.9479437512	-0.0687606671	-3.3072273257

TS4-11
Gas phase Energy: -852.43844651097 hartrees
Solvation Energy: -0.00995988352 hartrees
Zero Point Energy: 148.974 kcal/mol
Free Energy: -31.108 kcal/mol

angstroms

atom	x	y	z
Pd1	0.0023010010	0.0127212915	-0.0169483069
N2	0.0132159276	-0.0009323852	2.0834542951
C3	1.1961562858	0.0584933407	2.7322085459
C4	1.2984676468	0.0384519217	4.1194089881
C5	0.1349430142	-0.0484379764	4.8832247424
C6	-1.0895475939	-0.1101620355	4.2199613331
C7	-1.1094359431	-0.0810178362	2.8285089975
H8	2.0739527152	0.1204345229	2.0980835131
H9	2.2772304976	0.0916545905	4.5852324769
H10	0.1815215054	-0.0664187507	5.9680099269
H11	-2.0249895335	-0.1778378494	4.7659492978
H12	-2.0400596154	-0.1191884426	2.2755127599
N13	2.2818644637	-1.0125813884	-0.4424774694
C14	2.7393654898	-2.1412592612	0.1190281232
C15	3.7208346046	-2.9429774324	-0.4614582577
C16	4.2552366618	-2.5550316880	-1.6897404167
C17	3.7834702582	-1.3855859063	-2.2842390688
C18	2.7979199005	-0.6496886514	-1.6275160856
H19	2.2938982302	-2.4122911449	1.0740061653
H20	4.0516905188	-3.8482402550	0.0380683867
H21	5.0201239813	-3.1546169085	-2.1753806135
H22	4.1644785779	-1.0474133700	-3.2427435712
H23	2.3813456973	0.2519058986	-2.0668872551
H24	-1.5117522429	0.6086761685	-0.3209680267
O25	-0.2957253786	0.2378264258	-2.1396457828
C26	-1.4611816341	0.6896753362	-2.3290536360
O27	-2.2805857641	0.9430211163	-1.3831331061

C28	-1.9346214979	0.9470839651	-3.7431820149
H29	-1.1414363697	0.7465970462	-4.4639659969
H30	-2.7970722285	0.3086213156	-3.9577132628
H31	-2.2697509837	1.9843040831	-3.8339908974

TS1-16
Gas phase Energy: -852.41108053098 hartrees
Solvation Energy: -0.01723896017 hartrees
Zero Point Energy: 149.945 kcal/mol
Free Energy: -30.523 kcal/mol

angstroms

atom	x	y	z
Pd1	-0.1379551729	-0.1639527801	-0.0094945175
N2	-0.0634370399	-0.2145590312	2.0919333492
C3	0.7648830400	0.6585385216	2.7034012949
C4	0.7958359428	0.7870293799	4.0893050097
C5	-0.0510230427	0.0007769869	4.8680469831
C6	-0.9025420560	-0.9020771207	4.2314233969
C7	-0.8748616844	-0.9833548960	2.8436598088
H8	1.3993349462	1.2406783196	2.0378580800
H9	1.4771795070	1.4999821507	4.5413284594
H10	-0.0472637305	0.0863870134	5.9507496344
H11	-1.5769072083	-1.5387828636	4.7942756464
H12	-1.5116814002	-1.6782829549	2.3066895750
N13	-0.0582742062	-0.2029928624	-2.1116461727
C14	0.7777831167	0.6682664228	-2.7145539186
C15	0.8047443435	0.8161745949	-4.0983939419
C16	-0.0559692324	0.0522849103	-4.8842661515
C17	-0.9157410173	-0.8490632778	-4.2566951284
C18	-0.8822572109	-0.9509590776	-2.8703400156
H19	1.4206658609	1.2350123784	-2.0448757916
H20	1.4926661776	1.5272773132	-4.5432714551
H21	-0.0567483711	0.1543486831	-5.9655539824
H22	-1.6012248066	-1.4684603664	-4.8254056577
H23	-1.5253711005	-1.6455836265	-2.3404218654
H24	1.3514635967	-0.1974756978	-0.0049937066
C25	0.9485476517	2.7786946774	-0.0211697094
O26	-0.2742245590	2.4893597728	-0.0497053577
O27	1.9226844353	1.9533256233	0.0120959986
C28	1.3139970347	4.2734768837	-0.0084977497
H29	0.7495408678	4.8027547387	-0.7827331872
H30	1.0204643066	4.7097152515	0.9535351881
H31	2.3856366870	4.4257856096	-0.1549017964

TS21-22
Gas phase Energy: -1081.54602764238 hartrees

Solvation Energy: -0.01208320921 hartrees
Zero Point Energy: 189.626 kcal/mol
Free Energy: -36.804 kcal/mol

	angstroms		
atom	x	y	z
Pd1	0.2201021271	-0.2320367319	0.0456305614
N2	0.2840855920	-0.3174996244	2.1516665833
C3	1.2302969504	0.3456445569	2.8481538565
C4	1.2887732901	0.2988992305	4.2384202538
C5	0.3448640226	-0.4533230803	4.9354416060
C6	-0.6364855359	-1.1317056181	4.2130060935
C7	-0.6343882440	-1.0376120204	2.8253114881
H8	1.9324529000	0.9224577598	2.2530944173
H9	2.0666595210	0.8487624349	4.7578476810
H10	0.3701207205	-0.5076446258	6.0199822699
H11	-1.3966391084	-1.7251428697	4.7104360459
H12	-1.3867628641	-1.5304576080	2.2191197859
N13	0.3893428178	-0.2504393392	-2.0571676244
C14	1.4158403755	0.3612318730	-2.6828906938
C15	1.5398048911	0.3616154111	-4.0693438476
C16	0.5752254724	-0.2862527641	-4.8389737568
C17	-0.4905408122	-0.9093462256	-4.1903968839
C18	-0.5486656157	-0.8682745743	-2.8011051433
H19	2.1291048722	0.8623740645	-2.0365121877
H20	2.3826534352	0.8671120447	-4.5290715067
H21	0.6491295609	-0.3015888636	-5.9225407308
H22	-1.2705941601	-1.4193660733	-4.7459899147
H23	-1.3662175060	-1.3204609122	-2.2499053703
H24	1.6444160044	0.2869351249	0.0963994074
O25	-2.1864866257	-0.2030181132	0.0077576438
C26	-2.7306781410	0.9036353975	0.1065318407
O27	-2.1264020893	2.0650984170	0.1530822436
C28	-4.2363853789	1.0347905044	0.1882097350
H29	-4.6009315896	1.6099957921	-0.6685382888
H30	-4.7007082784	0.0488515621	0.1969328914
H31	-4.5116801501	1.5900162745	1.0895026978
O32	2.4067069988	1.8625081847	0.1659121062
C33	1.5774333809	2.8161252832	0.0276958316
O34	0.3225449927	2.7395333595	-0.0698570408
C35	2.1701023996	4.2302890540	-0.0143816266
H36	1.7119593572	4.8025738732	-0.8262524591
H37	1.9264817094	4.7471159091	0.9209325559
H38	3.2548412271	4.2040754076	-0.1333385448
H39	-1.1087201991	2.0857668113	0.0743394853